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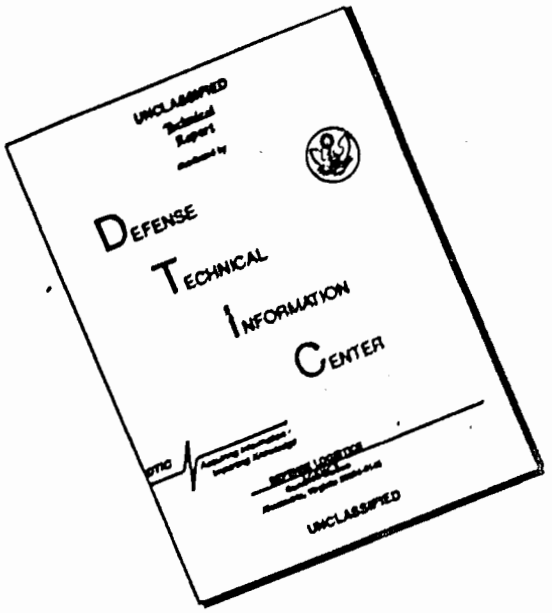

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THEORY OF SHALLOW DONOR STATES WITH A STRONG CENTRAL CELL PERTURBATION*

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A new theory for shallow donor states with a strong central cell perturbation is presented. The impurity wave function is expanded in terms of generalized Wannier functions, equivalent to the eigenfunctions of the periodic lattice with the strong central cell perturbing potential. The single unknown parameter of this theory can be fitted by comparison with the observed binding energy. The theory is applied to the impurity states of As, P and Sb in Silicon. The Fermi contact constants for the Si^{29} lattice nuclei surrounding the impurity are calculated and compared to the ENDOR experiments of Hale and Mieher and to recent calculations, using a different method, by Ivey and Mieher. ~~We also offer~~ some elucidations of the theory of Ivey and Mieher are offerred. In contrast to the conclusions of these authors, ~~we find~~ it is found that a suitable form of the Effective Mass Theory can account for the observations within an accuracy of about 10-15%.

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I. INTRODUCTION

Much theoretical work has been done on the calculation of impurity energy levels and wave functions. The shallow donor energy levels in Silicon were qualitatively understood very early in terms of a hydrogenic model called the Effective Mass Theory (EMT)[1], in which the impurity wave function is expanded in terms of the Bloch waves of the perfect crystal. For sufficiently localized perturbing potentials, the Koster-Slater theory[2-4], in which the impurity wave function is expanded in terms of Wannier functions[5], is often used. Recently pseudopotential theory has been adopted to calculate the impurity energy levels and wave functions. Pantelides and Sah[6], as well as Schechter[7-9], have reformulated the EMT in terms of a pseudopotential scheme. However, in both cases, the use of the EMT was logically not justified because, although their pseudopotentials were weak, they were not slowly varying on the scale of the lattice cell dimension.

Approximately simultaneously with this research, a detailed, many-band calculation of impurity states in Silicon was undertaken by Ivey and Mieher (I-M)[10]. Their calculation was very thorough and was the most comprehensive analysis of the wave functions for shallow donor states in Silicon to date. Their results were in much better agreement with the experimental data, from the ENDOR experiments of Hale and Mieher[11-12], than those of any previous work. I-M compared their results with those given by the EMT and concluded that the calculation of these shallow donor impurity wave functions is outside the realm of the EMT. Since we have just completed a calculation of these donor wave functions,

using a generalized form of the EMT, we will conclude with some comments on their method and conclusions.

We believe that the present approach succeeds for the first time in yielding a logically correct one-band theory of shallow impurity states with a strong central cell perturbation. The effects of both the deviations of the potential from Coulombic form and the important interband effects produced by the central cell potential are describable by generalized Wannier functions (GWF) belonging to a single band.[13]

From a theoretical point the shallow impurity states in Silicon are not a particularly ideal case for the application of this theory since, due to the small energy gap between the valence and conduction bands, the Wannier functions are not very highly localized. The reason why these systems were nevertheless chosen was that all the necessary information about the structure of the conduction bands and the impurity states was known. Another class of systems that might be successfully treated by this approach are color centers in alkalai halides.

II. GENERALIZED WANNIER FUNCTION THEORY OF IMPURITY STATES WITH APPLICATIONS TO DONOR STATES IN SILICON

A. Formulation of the Theory

When a shallow donor impurity is introduced into a perfect lattice, the Hamiltonian for the electrons may be written as

$$H = H_0 + U \ , \tag{1}$$

where H_0 is the Hamiltonian of the perfect lattice and U is the perturbation due to the impurity, which has the asymptotic form,

$$U(\vec{r}) \longrightarrow - \frac{e^2}{Kr} \ . \tag{2}$$

(κ is the static dielectric constant of the host lattice.) The wave functions satisfy the differential equation,

$$(H - E)\Psi = 0. \tag{3}$$

The ground state wave function may be expanded in terms of the perfect lattice Wannier functions, $a^{o}_{n,s}$, as in the Koster-Slater theory[2-4],

$$\Psi = \sum_{n,s} c_{n,s}\, a^{o}_{n,s} , \tag{4}$$

where n is a band index and s is a site index. The coefficients satisfy the set of difference equations,

$$\sum_{n',s'} (a^{o}_{n,s} \,|H|\, a^{o}_{n',s'})\; c_{n',s'} = E\, c_{n,s} . \tag{5}$$

If the potential is a smoothly varying function of $\vec{r}$, the matrix elements of H will be essentially zero unless the band indices are the same, in which case (5) reduces to a one-band set of equations. However, in the shallow donor impurity problem the potential is not smoothly varying in the central region so that solution of the set of equations (5) becomes a very difficult many-band problem.

In order to circumvent this difficulty we expand the wave function in terms of an appropriate set of generalized Wannier functions (GWF), which are constructed so as to insure that the matrix elements of H between these functions is negligible unless their band indices are the same. We write the total potential as the sum of two terms

$$U(\vec{r}) = U_1(\vec{r}) + U_2(\vec{r}) , \tag{6}$$

where $U_2(\vec{r})$ is a smoothly varying function of $\vec{r}$ for all $\vec{r}$, which reduces to the form given by (2) in the asymptotic region and is smoothly continued throughout the central region in an arbitrary way. By smoothly varying we mean that $U_2(\vec{r})$ is essentially constant over the range of a Wannier function. From our requirements on $U_2(\vec{r})$, $U_1(\vec{r})$ is necessarily short range.

In a manner similar to that described in a recent paper by the author and W. Kohn[4], we can construct the GWF, $a_{n,s}$, which are equivalent to the eigenfunctions of

$$H_1 = H_0 + U_1 , \tag{7}$$

in which the short range potential U_1 is included. These GWF are orthonormal,

$$(a_{n,s} | a_{n',s'}) = \delta_{n,n'} \delta_{s,s'} . \tag{8}$$

They have the same degree of localization as the perfect lattice Wannier functions and approach them exponentially for lattice sites distant from the impurity site. Their construction insures that the matrix elements of H_1 between them is zero unless their band indices are the same. Since U_2 is required to be smooth, all of its off-diagonal matrix elements in both n and s will be negligible.

We now write the ground state impurity wave function as a linear combination of the GWF associated with the lowest band (and drop the band index),

$$\Psi(\vec{r}) = \sum_s c_s \, a_s(\vec{r}) , \tag{9}$$

where the c_s's satisfy the set of difference equations

$$\sum_{s'} (a_s|H|a_{s'}) c_{s'} = E\, c_s . \tag{10}$$

In the region far from the impurity the GWF are the same as the perfect lattice Wannier functions; $U_1(\vec{r})$ is zero; and $U_2(\vec{r})$ is given by (2). Therefore, the Hamiltonian matrix element can be written as

$$(a_s|H|a_{s'}) = (a_s^0|H_0|a_{s'}^0) - \frac{e^2}{\kappa r_s}\,\delta_{s,s'} - \lambda_{s,s'} , \tag{11}$$

where $\vec{r}_s$ is the location of the midpoint of the s^{th} Wannier function and the matrix elements $\lambda_{s,s'}$, describing the effect of the short range potential, are, for the moment, unknown parameters. We assume

$$\lambda_{s,s'} = 0 , \tag{12}$$

except for Wannier functions near the impurity.

B. Application to Donor States in Silicon

We will now consider a shallow donor impurity in Silicon. The four conduction bands in this crystal are connected. As was shown in a paper by Kohn[15], in order to obtain a localized set of antibonding Wannier functions, one must use all of the eigenfunctions associated with these bands. Each Wannier function is labelled by a site index j and a bond index m, where m refers to one of the four bonds associated with the atom at site j.

The ground state wave function transforms according to the symmetric representation A_1 of the crystal point group T_d. Hence, those expansion coefficients which are equivalent under the operations of the group T_d are equal. This leads one to define a new set of orthonormal basis functions, a_s, which are proportional to the sum of all Wannier functions which are

equivalent under the operations of the group T_d. The wave function is then written as in (9), where the c_s's are the coefficients associated with this new set of basis functions and satisfy a set of difference equations of the form (10).

In the asymptotic region the difference equations are the same as those in the Koster-Slater theory[2-4], which can easily be shown to reduce to the EMT. Hence the coefficients c_s may be taken to be approximately equal to the values which would be obtained from the EMT for s large enough[16].

Because of the short range nature of $U_1(\vec{r})$ we assumed that

$$\lambda_{s,s'} = \lambda I_{s,s'}, \tag{13}$$

where

$$I_{s,s'} = \delta_{s,1}\,\delta_{s',1}\ . \tag{14}$$

The matrix elements of H_o between the perfect lattice Wannier functions are related to the Bloch energies $E^o_{n,\vec{k}}$ and were determined by a fit to the Silicon energy conduction bands.

The single parameter λ was determined by fitting the experimental binding energy, E_{exp}. If we define

$$K_{s,s'} = (a^o_s|H_o|a^o_{s'}) - \frac{e^2}{\kappa r_s}\,\delta_{s,s'} - E_{exp}\,\delta_{s,s'}, \tag{15}$$

equation (10) may be written as

$$\sum_{s'}(K_{s,s'} - \lambda I_{s,s'})c_{s'} = 0, \tag{16}$$

where λ may be regarded as an unknown eigenvalue, given by the stationary

expression

$$\lambda = \frac{\sum_{s,s'} c_s K_{s,s'} c_{s'}}{\sum_{s,s'} c_s I_{s,s'} c_{s'}} , \qquad (17)$$

which is a minimum for the correct c_s's. Because of computer limitations we were only able to determine 45 unknown coefficients. We assumed that the rest were given by their EMT values. For the impurities Sb, P, and As, the parameters λ were determined to be .187, .219, and .281 eV respectively. We found that the coefficients for the Wannier functions far from the impurities differed very little from their EMT values.

The Fermi contact constants, a_j, at the Si^{29} nuclei surrounding the impurities (P, As, Sb) have been determined from ENDOR experiments performed originally by G. Feher[17] and most recently and completely by Hale and Mieher[11]. They are proportional to the wave function density at the j^{th} site[11],

$$|\Psi(R_j)|^2 = 1.523 \times 10^{-2} |\tfrac{1}{3} a_j| \text{ Å}^{-3} , \qquad (18)$$

where $\frac{1}{3} a_j$ is expressed in MHz. When the crystal orientation in the magnetic field is varied, the angular dependence of the ENDOR signal allows one to recognize which signals belong to nuclei on sites of the types $\langle aaa \rangle$, $\langle 00a \rangle$, and $\langle aab \rangle$. A knowledge of the wave function at the lattice sites enables one to match observed experimental lines to specific lattice sites.

In the calculation of the Fermi contact constants we used orthogonalized, directed tetrahedral orbitals for the Wannier functions. Our

results, along with those of I-M[10] and the experimental values[11], are presented in Tables I and II. We agreed with I-M on the matching of slightly more than half of the observed lines with specific lattice sites[18]. Agreement with I-M for sites of the type ⟨aaa⟩ and ⟨00a⟩ was perfect. For sites of the other type, the matching procedure is more ambiguous, and we have less confidence in the assignments offered by either I-M or by us. The overall agreement of our values with experiment is slightly worse than that of I-M, presumably because of the relatively poor localization of the Silicon Wannier functions.

III. SOME COMMENTS ON THE IVEY-MIEHER METHOD AND CONCLUSIONS

Ivey and Mieher[10] use a one-step iteration to calculate the pseudo impurity wave function, which satisfies the equation

$$(H_o + U_p - E)\Psi_p = 0, \tag{19}$$

where U_p is the pseudopotential and Ψ_p is expanded in terms of the pseudo Bloch waves with coefficients $A_n(\vec{k})$. H_o is the Silicon lattice Hamiltonian, which is highly anisotropic. To lowest approximation they use a function $\Psi_c(\vec{r})$ which has spherical symmetry. To allow for the anisotropy of the wave function due to the anisotropy of H_o and to obtain the components of the wave function associated with other branches of the conduction and valence bands, they then solve

$$(H_o - E)\Psi_p = - U_p \Psi_c \tag{20}$$

This is not a consistent iteration technique for obtaining the anisotropy, and therefore we decided to do a simple calculation in order to obtain an estimate of the errors inherent in this procedure. On the basis of this calculation we estimate that the anisotropy obtained from (20) is up to 30% too small.

We considered the case of a Silicon lattice effective Hamiltonian with a small anisotropy,

$$H_o = -\frac{\hbar^2}{2m^*}\nabla^2 + H_o' , \tag{21}$$

where

$$H_o' = -\lambda\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial z^2} - \frac{1}{3}\nabla^2\right) . \tag{22}$$

The parameter λ is a measure of the anisotropy in the Hamiltonian. The full effective mass wave function satisfies

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 + H_o' - \frac{e^2}{\kappa r} - E\right)\psi = 0. \tag{23}$$

The zeroth order wave function ψ_o and energy E_o satisfy the hydrogen atom Schrödinger equation. The first order correction to the energy is zero, and the first order correction to the wave function is determined by

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\kappa r} - E\right)\psi_1 = -H_o'\psi_o . \tag{24}$$

If we followed the I-K procedure of equation (20), we would obtain a first order correction to the wave function which satisfies

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 - E\right)\psi_1 = -H_o'\psi_o , \tag{25}$$

instead of the correct equation (24). The term $-e^2/\kappa r$ omitted on the left hand side of equation (25) is of the same order as the terms kept. Although the solutions to (24) and (25) agree for $\vec{r}$ near zero (because of the d-character of ψ_1), their ratio decreases to about 70% by the time $r \sim 3c$, where c is the Silicon lattice constant.

Thus we see that use of the procedure (20) introduces significant errors into those parts of the wave function which are associated with the two lowest conduction bands. On the other hand one can verify that the I-M equation (20) does give a good approximation for the parts of Ψ_p associated with the other branches of the conduction and valence bands.

In their abstract I-M state that the EMT restricts itself to a single band and to conduction-band-minima Bloch functions. We would like to point out that: (1) When an energy band minimum is near a band edge, the EMT must employ an extended zone scheme which, in a reduced zone scheme, leads to inclusion of more than one band. (2) The EMT assures that the wave functions are made up of wave packets of Bloch functions, $\Phi_{\vec{k}}$, localized near the conduction band minima. This is, in fact, confirmed by the results of I-M, as they find that the bands excluded in the (extended zone) EMT contribute typically only about 10% to the Fermi contact constants.

There are <u>two</u> levels of approximation in the EMT. On the first, more accurate, level of approximation the Fourier transform, $F_j(\vec{r})$, of the Bloch wave coefficients $A(\vec{k})$ (taken with respect to the conduction band minimum, $\vec{k}_j$) satisfies an anisotropic hydrogenic type differential equation. Thus $A(\vec{k})$ is real and even in the components of $(\vec{k}-\vec{k}_j)$. On the second, less accurate, level of approximation the impurity wave function at the lattice sites $\vec{R}_\ell$ is written as

$$\Psi(\vec{R}_\ell) = \sqrt{\frac{1}{\mathcal{N}}} \sum_j F_j(\vec{R}_\ell)\Phi_{\vec{k}_j}(\vec{R}_\ell), \qquad (26)$$

which is based on the assumption that the periodic part of the Bloch wave, $u_{\vec{k}}(\vec{R}_\ell)$ may be replaced by $u_{\vec{k}_j}(\vec{R}_\ell)$ because of the localization of

$A(\vec{k})$ near $\vec{k}_j$. In fact, for Silicon this is not a good approximation for the lattice sites which do not have inversion symmetry. Hence this second level of approximation cannot be expected to hold for these sites.

I-M calculate a function F_j^C defined by

$$\sqrt{\frac{1}{\Omega}}\, F_j^C(\vec{R}_\ell)\Phi_{\vec{k}_j}(\vec{R}_\ell) = \sum_{\vec{k}}^{j} A(\vec{k})\,\Phi_{\vec{k}}(\vec{R}_\ell)\ , \qquad (27)$$

which they compare with the EMT function $F_j(\vec{R}_\ell)$. (The superscript j on the summation indicates that the summation is performed over the one-sixth of $\vec{k}$-space associated with the j^{th} conduction band minimum and extending through the first two Brillouin zones.) They find that, for many of the lattice sites which do not have inversion symmetry, F_j^C has a large imaginary part. They conclude that their results are not compatable with the EMT. In fact, the main inconsistency is with the second, less accurate, level of the EMT since for most of the lattice sites with inversion symmetry the imaginary part of F_j^C is small. The main exception to this statement is F_z^C for the site (0,0,c), which I-M report to have an imaginary part which is about 30% of its real part. Since we were surprised by this, we also calculated F_z^C for this site using our wave function. We found that the imaginary part was about 20% of its real part and that most of it (about 15%) was due to a real term in $A(\vec{k})$ which was odd in $(\vec{k}-\vec{k}_j)_z$, and which arose from the odd part of the potential matrix element $(\Phi_{\vec{k}}|U|\Psi)$. Thus this large imaginary part does not signify a breakdown of the EMT.

We believe that a comparison of our work and that of I-M is useful

for the understanding of shallow donor states and specifically to the application of the EMT to this problem. We found that by using generalized Wannier functions and by matching a good inner region solution to the asymptotic EMT solution (which only used the first level of approximation), we were able to calculate quantitative impurity state wave functions, including strong central cell effects.

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FOOTNOTES

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13. For a composite band one must include all branches. See footnote 15.

14. W. Kohn and J. R. Onffroy, Phys. Rev. 8, B2485 (1973).

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16. The exact form of these coefficients is given in the thesis of J. R. Onffroy, UCSD, 1976.

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18. A more detailed discussion of the matching procedure may be found in the thesis of J. R. Onffroy, UCSD, 1976.

Table I. Calculated and Experimental Values of the Fermi Contact Constants, $1/2\, a_j$, for Lattice Shells at Sites on the ⟨001⟩ and ⟨111⟩ Axes.

Shell	Impurity	Expt.[11] $1/2\, a_j$ (MHz)	Lattice Site (c/4) (Onffroy & I-M)	$1/2\, a_j$ (MHz)	
				Onffroy	I-M[10]
A	As	3.860	(0, 0, 4)	2.818	3.803
	P	2.981		2.517	2.924
	Sb	3.101		2.357	2.554
K	As	.758	(0, 0, 8)	.781	.649
	P	.663		.708	.570
	Sb	.629*		.667	.529
C	As	2.037	$(3, 3, \bar{3})$	1.168	1.991
	P	1.649		1.063	1.477
	Sb	1.397		1.004	1.267
J	As	.694	(5, 5, 5)	.752	.657
	P	.739		.789	.686
	Sb	.761*		.788	.685
H	As	.801	$(4, 4, \bar{4})$	.694	.943
	P	.689		.658	.787
	Sb	.703		.632	.713
O	As	.739	(4, 4, 4)	.685	.775
	P	.598		.632	.652
	Sb	.670		.600	.593
N	As	.607	$(7, 7, \bar{7})$	.488	.647
	P	.612		.530	.634
	Sb	.629*		.538	.617
E	As	.642	(1, 1, 1)	2.748	.003
	P	.270		1.216	.018
	Sb	.293		.781	.045

*This data was missing in Reference 11 and was later determined by I-M[10].

Table II. Calculated and Experimental Values of the Fermi Contact Constants, $1/2\,a_j$, for Lattice Shells with Position Vectors of the Form (a,a,c).

Shell	Impurity	Expt.[11] $1/2\,a_j$ (MHz)	Onffroy Lattice Site (c/4)	Onffroy $1/2\,a_j$ (MHz)	I-M[10] Lattice Site (c/4)	I-M[10] $1/2\,a_j$ (MHz)
B	As	3.000	(0, 4, 4)	2.984	(0, 4, 4)	2.701
	P	2.254		2.348		1.922
	Sb	1.833		2.081		1.609
D	As	1.292	(2, 2, 4)	1.154	(3, 3, $\bar{7}$)	1.242
	P	1.117		.885		1.008
	Sb	1.003		.776		.901
F	As	1.121	(2, 2, $\bar{4}$)	1.006	(1, 3, 3)	1.295
	P	.840		.799		.788
	Sb	.504*		.712		.606
G	As	.806	(3, 3, $\bar{7}$)	.859	(3, 7, $\bar{7}$)	.861
	P	.764		.810		.774
	Sb	.761		.776		.725
I	As	.718	(2, 2, 8)	.720	(2, 2, $\bar{8}$)	.646
	P	.685		.692		.589
	Sb	.643		.669		.556
L	As	.741	(0, 2, 2)	.632	(2, 2, 4)	.716
	P	.582		.486		.537
	Sb	.525*		.426		.462
M	As	.777	(1, 3, 3)	.633	(2, 2, $\bar{4}$)	.819
	P	.612		.512		.612
	Sb	.559		.459		.528
P	As	.696	(2, 2, $\bar{8}$)	.666	(2, 2, 8)	.627
	P	.662		.651		.573
	Sb	.629		.633		.541
Q	As	.566	(1, 1, 5)	.498	(1, 1, 5)	.545
	P	.524		.449		.447
	Sb	.387		.422		.403
R	As	.428	(1, 1, $\bar{3}$)	.436	(1, 7, 7)	.449
	P	.379		.217		.378
	Sb	.332		.150		.344
S	As	.377	(5, 5, 9)	.494	(2, 2, $\bar{12}$)	.411
	P	.410		.523		.424
	Sb	.425*		.525		.422
T	As	.364	(2, 2, 12)	.476	(2, 2, 12)	.401
	P	.398		.502		.415
	Sb	.425*		.504		.412
U	As	.338	(2, 2, $\bar{12}$)	.476	(5, 5, 9)	.396
	P	.383		.502		.424
	Sb	.425*		.504		.428
X	As	.242	(1, 5, 5)	.271	(1, 5, 5)	.337
	P	.317		.343		.398
	Sb	.437		.366		.418
W	As	*	(5, 9, 9)	.275		
	P	.328		.309		
	Sb	*		.318		
*	As	*	(3, 7, $\bar{7}$)	.573		
	P	*		.593		
	Sb	*		.591		
	As		(1, 7, 7)	.201		
	P			.216		
	Sb			.218		

*These values were not present in the original data. See reference 18 for further details.

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A new theory for shallow donor states with a strong central cell perturbation is presented. The impurity wave function is expanded in terms of generalized Wannier functions, equivalent to the eigenfunctions of the periodic lattice with the strong central cell perturbing potential. The single unknown parameter of this theory can be fitted by comparison with the observed binding energy. The theory is applied to the impurity states of As,P and Sb in Silicon. The Fermi contact constants for the Si^{29} lattice nuclei surrounding the impurity are calculated and compared to the ENDOR experiments of Hale and Mieher and to recent calculations, using a different method, by Ivey and Mieher. We also offer some elucidations of the theory of Ivey and Mieher. In contrast to the conclusions of these authors, we find that a suitable form of the Effective Mass Theory can account for the observations within an accuracy of about 10-15%.

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AB

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
SHALLOW DONOR STATES						
GENERALIZED WANNIER FUNCTIONS						
EFFECTIVE MASS THEORY						
HYPERFINE INTERACTIONS						